| |
|---|
| AD NUMBER |
| **AD839359** |
| NEW LIMITATION CHANGE |
| TO<br>**Approved for public release, distribution unlimited** |
| FROM<br>**Distribution authorized to U.S. Gov't. agencies and their contractors; Critical Technology; JUL 1968. Other requests shall be referred to Department of the Army, Fort Detrick, Attn: Technical Release Branch, Frederick, MD 21701.** |
| AUTHORITY |
| **AMXFD ltr, 9 Feb 1972** |

AD839359

TRANSLATION NO. 1060

DATE: 17 July 1968

DDC AVAILABILITY NOTICE

Reproduction of this publication in whole or in part is prohibited. However, DDC is authorized to reproduce the publication for United States Government purposes.



STATEMENT #2 UNCLASSIFIED

This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of Dept. of Army, Fort Detrick, ATTN: Technical Release Branch/ TID, Frederick, Maryland 21701

...ols and each ...tionals may be

DEPARTMENT OF THE ARMY
Fort Detrick
Frederick, Maryland

Attn: Tech. Library

Best
Available
Copy

T-163-6

Translation #1060

THEORETICAL CHEMISTRY. -Electronic conduction in DNA and in the DNA-$Mg^{2+}$ complex. Note (*) of Madame Andree Goudot, presented by Prince Louis de Broglie. Compt. Rend. 255:3420-3422, 1962.

Calculation of energy levels of free electrons in the molecules; adenin-thymin, Guanidin-cytosin and adenin-$Mg^{2+}$ -thymin, guanidin-$Mg^{2+}$ -cytosin. The results show debased levels in DNA and DNA-$Mg^{2+}$. Furthermore there is a conduction band in DNA-$Mg^{2+}$.

It has been experimentally shown that the conductibility of a solution DNA-$Mg^{2+}$ is greater than that of an aqueous solution of pure DNA (1). On the other hand the electrical properties (2) of DNA have been studied in the form of DNA-$Na^{+}$.

In the desoxyribonucleic acid the purin-pyrimidin molecules form adenin-thymin and guanidin-cytosin planes which are parallel and which are separated by a distance of only 3.4 Å. There can therefore be interaction between these plane molecules, and in particular a transfer of mobile electrons if molecular energy levels allow it. Whence the interest of this theoretical study of pure DNA and of the complex DNA-$Mg^{2+}$.

I. DNA. - Calculation of energy levels of mobile electrons and of charges for each of the adenin-thymin and guanidin-cytosin molecules. Those levels are within parallel planes, and may therefore be compared as to their value.

1° Adenin-thymin (AT). - The calculation of the delocalization energy shows that inside the AT molecule a charge neighboring that of two electrons runs from adenin onto thymin. This may be due to two CO groupings, which are strongly $\pi$ "acceptors" of thymin.

2° Guanidin-cytosin (GC) - In the GC molecule guanidin and cytosin each roughly preserve their respective charges.

3° Interactions inside DNA. - a. Occupied levels:

AT : 3.821; 3.690; 3.651; 3.436; 2.467; 2.321; 1.967 and 1.629;

GC : 3.701; 3.648; 3.390; 3.256; 2.604; 2.527; 2.467; 2.299; 1.759 and 1.322.

The AT and GC molecules have the same energy level (2.467) and this level is a degenerated energy level for the DNA molecule.

c. Lowest free level: for AT : 1.241 and for GC : 1.178.

The lowest free level of AT being situated below that of GC, if an excitation energy permits passage from the highest occupied level (that of GC : 1.322) to the lowest free level (that of AT : 1.241) there will be an electronic transfer from GC onto AT, but this transition cannot continue from TA onto GC, that is along the DNA molecule.

2. DNA-$Mg^{2+}$. - $Mg^{2+}$ yields octahedric hexavalent complexes. The pyrimidin-$Mg^{2+}$ purin is then a symmetry plane of the complex where $Mg^{2+}$ is connected with four atoms which were connected two-by-two with H connections in pure DNA. Thus, there can be as many metal cations as purin-pyramidin planes in the DNA molecule. The distance between the purin and the pyramidin does not undergo any great variation. In the DNA it is between 2.8 and 3 Å. And since the ion ray of $Mg^{2+}$ is 0.78 Å, we have: $Mg^{2+}$-O = 1.44 Å and $Mg^{2+}$ - N = 1.48 Å. Whence the distance purin-$Mg^{2}$-pyramidin is near 2.92 Å.

1° Adenin-$Mg^{2+}$-thymin (AT-$Mg^{2+}$) - As in the case of pure DNA a charge in the neighborhood of two electrons runs from adenin onto thymin.

The highest occupied level for DNA-$^{2+}$Mg (1.632) is very near that of DNA (1.629). But the lowest free level has come near the occupied levels. It is of 1.363 for DNA-$Mg^{2+}$ instead of 1.241 for DNA.

2° Guanidin-$Mg^{2+}$-cytosin (GC-$Mg^{2+}$). - Guanidin and cytosin preserve their own charges. The highest occupied level is the same (1.322). The lowest free level and the highest occupied level are getting nearer: 1.285 instead of 1.178.

3° Interactions inside DNA-$Mg^{2+}$. a. Occupied levels:

AT-$Mg^{2+}$ : 3.843; 3.699; 3.576; 3.479; 2.969; 2.310; 1.966 and 1.632.

GC-$Mg^{2+}$ : 3.797; 3.651; 3.425; 3.307; 2.672; 2.558; 2.467; 2.310; 1.767 and 1.322.

As in pure DNA there is in DNA-$Mg^{2+}$ a debased level (2.310) which is nevertheless situated a little higher.

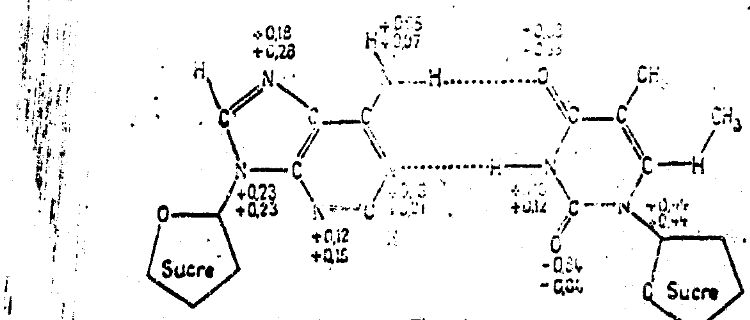
b. Lowest free level : for AT-$Mg^{2+}$ : 1.363 and for GC-$Mg^{2+}$ : 1.285.

If we compare the energy levels of free electrons for the purin-pyramidin planes, we have

| | AT-$Mg^{2+}$ | | GC-$Mg^{2+}$ |
|---|---|---|---|
| Highest occupied level ............ | 1.632 | and for | 1.332 |
| Lowest free level .................. | 1.363 | | 1.285 |

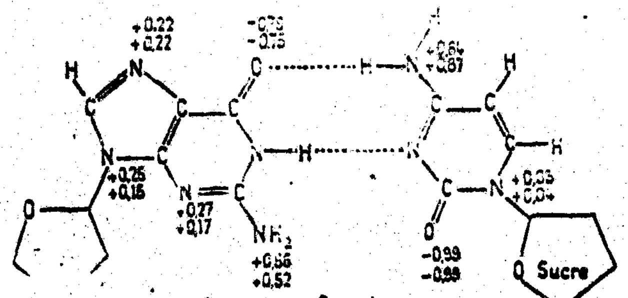
The lowest free level of AT-$Mg^{2+}$ has a lower energy than the highest occupied level of GC-$Mg^{2+}$. There may be a spontaneous transition from the highest occupied level of GC-$Mg^{2+}$ on the lowest free level of AT-$Mg^{2+}$ and vice-versa. Those levels are, furthermore, very near each other and form a narrow conduction band. That conduction band makes possible electronic conductibility through DNA-$Mg^{2+}$. The narrowness of this band makes it very specific. This characteristic makes it possible to explain certain electric properties of those complexes studied in vitro.

Charges. - If we consider charge distribution on each of the plane adenin-thymin- and guanidin-cytosin molecules, since both figures are placed in such a way that a pyrimidin is superposed to a purin and vice versa, we then see that the CO(-0.99) which is most charged with cystin is above the $NH_2$(+0.95) which is most positive of adenin. In return the CO(-0.83) grouping of thymin is situated just above the $NH_2$(+0.36) grouping of guanidin. That may allow Coulomb interactions between those groups (figures 1 and 2).




Adenin-Thymine

Fig. 1.




Guanidine-Cytosine

Fig. 2.

Sucre=sugar

[illegible] show: 1° either that the prop- [illegible] in vitro [illegible] compounds of DNA are not to [illegible] in vivo for pure DNA; 2° or that in vivo DNA forms an organo [illegible] complex and can then present the same properties as those found for those complexes in vitro.

(*) Séance of 5 December 1962.

(1) G. Zubay and L. Doty, Biochem. Bioph. Acta, 1958, p. 51.

(2) P. [illegible], C. Sadron and J. Polonsky, Proceedings, 250, 1960, p. 710; 251, 1960, p. 722.